

Haldane state with toroidal magnetic order

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We show that a simplified two-band model describing toroidal magnetic order in two-dimensional crystal is entirely equivalent to the well-known Haldane model of a honeycomb lattice in periodic internal magnetic field with zero total flux through the unit cell. Crystals with toroidal ordering can be considered as real physical systems which should exhibit topologically nontrivial state, predicted by Haldane, that is similar to the quantum Hall effect regime without any external magnetic field. Analogous description is formulated for quantum spin Hall effect without any spin-orbit interaction.

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Highly speculative model of a two-dimensional (2D) honeycomb lattice with two nonequivalent sublattices in periodic internal magnetic field, introduced by Haldane more than twenty years ago [1], directly predicts a new state of matter similar to the integer-valued Quantum Hall Effect (QHE) regime without any external magnetic field. It is presupposed in this Haldane model that internal magnetic-flux density with full symmetry of 2D lattice results in zero total flux through the unit cell. In the framework of the Haldane model, time-reversal invariance and 2D space-inversion symmetry are broken by the internal magnetic field and the non-equivalence of the sublattices, respectively. Tight-binding model [1] takes into account hopping matrix elements between nearest and second-neighbor sites (the nearest sites of a sublattice) and the periodic vector potential $\mathbf{A}(\mathbf{r})$ of the internal field is included into this model through the phase multipliers $\exp[i(e/\hbar c) \int \mathbf{A} d\mathbf{r}]$ of the hopping matrix elements. Thus, magnetic field in the model [1] becomes apparent through the vector potential in the phase factors of the wave functions similar to that in Bohm-Aharonov effect. Since internal magnetic field breaks time-reversal invariance, quasiparticle spectrum of the system with broken spatial inversion turns out to be nonsymmetric with respect to inversion of quasi-momentum, $\mathbf{k} \leftrightarrow -\mathbf{k}$. In addition, edge chiral fermion excitations, typical of the QHE regime, arise without partners of opposite chirality.

It should be noted that, simultaneously with and independently of the paper Ref.[1], Volovik [2, 3] has predicted and studied in detail the half-integer QHE in the A-phase of liquid helium-3 without both external magnetic field and rotation of the container.

In the QHE regime, quantizing external magnetic field normal to the plane of 2D crystal both transforms 2D metal into 2D insulator in which degenerated Landau levels play role of the bands of allowed states and also determine a direction of a drift of the cyclotron orbit center along the boundary of the crystal. Finite distance between the neighboring Landau levels and the absence of the backscattering in the edge chiral states result in a stability of the ground state of the QHE regime with respect to relatively weak structure perturbations. Com-

paratively weak internal periodic magnetic field in the Haldane model breaks time-reversal symmetry but in itself cannot create an insulating state in the form of a system of Landau levels like that in the QHE regime. However, as was also proposed by Haldane [1], sometimes the internal field could be associated with a magnetic ordered state with broken time-reversal invariance that might result in an insulating gap in the quasiparticle spectrum. Finite insulating gap and absence of backscattering could lead to a robust Haldane state similar to the QHE regime.

Thouless et al. [4] have shown that QHE regime differs from the conventional band insulating state by the integer-valued topological invariant: in the case of conventional (trivial) insulator, such a topological invariant turns out to be zero, $n = 0$ and edge states are absent; $n \neq 0$ may be referred to a *topological insulator*.

Edge states can also arise in the topological insulator with spin-orbit interaction which does not break time-reversal symmetry [5, 6]. Such edge states correspond to a transfer not of electric charge but of spin. Electrons with opposite spin projections move in opposite directions along crystal boundaries. This becomes apparent as spin quantum Hall effect [5, 6].

As it was pointed out by Haldane [1] and Volovik [3], topologically nontrivial insulating state with electric charge transfer over the edge states could be realized in 2D systems with magnetic order breaking time-reversal invariance of the Hamiltonian. However, one can conclude that such states have never been experimentally realized till now. In this Letter, we show that two-band model of excitonic insulator [7] with electron-hole pairing leading to toroidal magnetic order turns out to be equivalent to the Haldane model after very natural simplification. We believe the Haldane state can be realized just in 2D insulating crystals with toroidal magnetic order.

Such insulating crystals with spontaneous toroidal moment of the unit cell in the ordered phase are investigated theoretically long ago [8]. Since then, a great number of crystals and artificial 2D heterostructures with toroidal ordering were discovered [9] mainly because of their re-

relationship to the magnetoelectric effect.

Toroidal magnetic moment \mathbf{t} arises in the multipole expansion of the electrodynamic vector potential $\mathbf{A}(\mathbf{r})$ beginning with the second order term which can be presented as a sum of the contributions from the magnetic quadrupole and toroidal moments [10]. The toroidal part of the vector potential created by orbital currents at some distant point \mathbf{r} can be written as [9]

$$\mathbf{A}(\mathbf{r}) = \nabla(\mathbf{t} \cdot \nabla) r^{-1} + 4\pi \boldsymbol{\tau}(\mathbf{r}), \quad (1)$$

where

$$\boldsymbol{\tau}(\mathbf{r}) = \frac{1}{6c} [\mathbf{r} \times [\mathbf{r} \times \mathbf{j}(\mathbf{r})]] \quad (2)$$

is the toroidal moment density, $\mathbf{j}(\mathbf{r})$ is the orbital electric current density. Nonzero toroidal moment corresponds to a special distribution of orbital currents in Eq. (2). As a classical example, one can consider the so-called *poloidal* currents flowing through a solenoid that is bent into a torus.

One can imagine that all orbital currents are shrunk into the origin of coordinates [9]. Then the toroidal moment density (1) should be written as $\boldsymbol{\tau} \rightarrow \mathbf{t} \cdot \delta(\mathbf{r})$. The first term in Eq. (1) can be eliminated by appropriate gauge transformation so that the vector potential takes the form $\mathbf{A}(\mathbf{r}) = 4\pi \boldsymbol{\tau}(\mathbf{r})$.

It should be noted that toroidal moment can be created not only by persistent orbital currents but also by an appropriate configuration of magnetic dipole moments, such as head-to-tail arrangement of spins [9].

One can see that the toroidal contributions into both vector potential and magnetic flux density $\mathbf{B} = \text{rot} \mathbf{A}$ turn out to be localized inside a bounded domain of the real space in which toroidal moment density is nonzero. In the case of crystalline solid, such a domain is the unit cell so that both vector potential and magnetic flux density should be periodic functions with basic periods of the solid similar to that proposed in the Haldane model.

Since toroidal moment density $\boldsymbol{\tau}(\mathbf{r})$ is t -odd polar (\mathbf{r} -odd) vector, the mean field order parameter originating from toroidal ordering should change sign upon both time reversal and spatial inversion. As direct product of electric and magnetic field strengthes has the same symmetry toroidal order may be apparent as a linear magneto-electric effect. Corresponding contribution into the free energy of the form $F_{me} = -\alpha_{ik} E_i H_k$ where α_{ik} is a magneto-electric tensor. Magnetic field induced electric polarization and electric field induced magnetization are determined by this tensor as $P_i = \alpha_{ik} H_k$ and $M_i = \alpha_{ki} E_k$, respectively.

From the symmetry consideration, magneto-electricity should be one of the distinctive properties of the toroidal ordered state [9]: $\mathbf{P} = -[\mathbf{t} \times \mathbf{H}]$, $\mathbf{M} = [\mathbf{t} \times \mathbf{E}]$. Magneto-electric tensor can be decomposed into a pseudoscalar, a polar vector and a symmetric traceless tensor. Thus,

non-diagonal components of the magneto-electric tensor should be nonzero and antisymmetric, $\alpha_{ik} = -\alpha_{ki}$ [11].

The bulk adiabatic magneto-electric tensor determines the surface Hall impedance in a magneto-electric crystal [12], $R_H^{-1} = c n_i \alpha_{ik} n_k$, where c is light velocity. This thermodynamic relation is used in Ref. [1] to calculate quantized Hall conductivity σ_{xy} .

A rise of the toroidal ordering can be a result of an electron phase transition. It is convenient to describe such a transition in the framework of the model of the excitonic insulator with high-temperature (more symmetric) phase being 2D semimetal with equally centered isotropic electron and hole bands [8].

Bloch Hamiltonian of such two-band semimetal can be written as

$$\hat{H}_{\mathbf{p}} = \varepsilon_+(\mathbf{p}) \hat{\tau}^0 + \varepsilon_-(\mathbf{p}) \hat{\tau}^3 + (\boldsymbol{\gamma} \mathbf{p}) \hat{\tau}^2, \quad (3)$$

where $\hat{\tau}^0$ is the unit matrix, $\hat{\tau}^{1,2,3}$ are the Pauli matrixes, $2\varepsilon_{\pm}(\mathbf{p}) = \varepsilon_1(\mathbf{p}) \pm \varepsilon_2(\mathbf{p})$, $\varepsilon_s(\mathbf{p})$ is electron dispersion in the band s (electron energy is counted from the chemical potential), $\boldsymbol{\gamma} = \mathbf{p}_{12}/m$ is a real vector, \mathbf{p}_{12} is interband matrix element of momentum, m is electron mass. Note that $\mathbf{p}_{12} \neq 0$ when, in particular, the bands of the semimetal are formed by the hybrid states of different parity, for example, s and p states.

Fermi contour (FC), that is a boundary separating filling and vacant states in the electron and hole bands, is determined by the Fermi momentum \mathbf{p}_F . In the case of isotropic bands the FC is a circle with radius p_F . One can choose p_1 -axis along the vector $\boldsymbol{\gamma}$. For low-energy elementary excitations a deviation \mathbf{k} of quasimomentum from the Fermi momentum \mathbf{p}_F is small. Therefore, in the first approximation, one can replace the quasimomentum \mathbf{p} with \mathbf{p}_F in the non-diagonal terms of Hamiltonian (3) whereas the diagonal terms depend on \mathbf{k} directly because energies $\varepsilon_1(\mathbf{p})$ and $\varepsilon_2(\mathbf{p})$ are counted from the chemical potential.

Hamiltonian (3) is characterized by gapless anisotropic quasiparticle spectrum

$$E_{1,2}(\mathbf{k}) = \varepsilon_{\pm}(\mathbf{k}) \pm \sqrt{\varepsilon_-^2(\mathbf{k}) + (\boldsymbol{\gamma} \mathbf{p}_F)^2}, \quad (4)$$

which is symmetrical with respect to quasimomentum inversion, $\mathbf{k} \rightarrow -\mathbf{k}$.

To obtain both time-reversal and space-inversion symmetries to be broken one can consider the low-temperature ordered phase originating from electron-hole pairing resulting in nonzero toroidal moment. The order parameter is determined by an anomalous average $\langle \hat{c}_{1\mathbf{p}\sigma}^\dagger \hat{c}_{2\mathbf{p}\sigma'} \rangle$ corresponding to singlet ($\sigma = \sigma'$) or triplet pairing of electron and hole belonging to different bands. Here, $\hat{c}_{s\mathbf{p}\sigma}$ annihilates electron with quasimomentum \mathbf{p} and spin σ in the band $s = 1, 2$.

It is well known that orbital and spin current states corresponding to singlet and triplet electron-hole pairing,

respectively, can result in the ordered states with pure imaginal order parameter [13].

We restrict ourselves to the case of singlet electron-hole pairing resulting in a pure imaginal order parameter $i\Delta(\mathbf{k})$ where $\Delta(\mathbf{k})$ is a real function of quasimomentum \mathbf{k} . In such a case, toroidal order arises from poloidal charge currents. To associate the order parameter with the toroidal moment one should use the relation $\mathbf{t} = \gamma\Delta$ following from the interrelation between the charge current density and toroidal moment of the unit cell [14].

The singularity in the electron-hole pairing channel that could lead to the insulating ordered state at low temperature can arise under nesting of electron dispersion, $\varepsilon_1(\mathbf{k}) = -\varepsilon_2(\mathbf{k}) \equiv \varepsilon(\mathbf{k})$. We suppose that such a condition is fulfilled in a vicinity of the FC. Then the mean field Bloch Hamiltonian corresponding to singlet electron-hole pairing with a rise of a toroidal magnetic moment of the unit cell and pure imaginal order parameter $\Delta(\mathbf{k})$ takes the form

$$\hat{H}_{\mathbf{k}} = \hbar(\mathbf{v}_F\mathbf{k})\hat{\tau}^3 + [(\gamma\mathbf{p}_F) + \Delta(\mathbf{k})]\hat{\tau}^2, \quad (5)$$

where electron dispersion is presented by linear function of quasimomentum, $\varepsilon(\mathbf{k}) = \hbar(\mathbf{v}_F\mathbf{k})$. Here, \mathbf{v}_F is Fermi velocity. Later on, we restrict ourselves to the case of isotropic (*s*-wave) toroidal order parameter $\Delta = \text{const}$.

The spectrum of the high-temperature phase, when $\Delta = 0$,

$$E_{1,2}(\mathbf{k}) = \pm\sqrt{\hbar^2(\mathbf{v}_F\mathbf{k})^2 + (\gamma\mathbf{p}_F)^2}, \quad (6)$$

turns out to be gapless because of the fact that $\gamma\mathbf{p}_F = 0$ for two antipodal directions of the p_2 -axis. Two points on the FC corresponding to such directions form two Dirac cones with linear dispersion at small \mathbf{k} .

In the low-temperature phase, when $\Delta \neq 0$, quasiparticle spectrum corresponding to Bloch Hamiltonian (5) becomes gapped,

$$E_{1,2}(\mathbf{k}) = \pm\sqrt{\hbar^2(\mathbf{v}_F\mathbf{k})^2 + (\gamma\mathbf{p}_F + \Delta)^2}. \quad (7)$$

Similar to the Haldane model [1], the spectrum turns out to be asymmetric with respect to $\mathbf{k} \rightarrow -\mathbf{k}$: $E_{1,2}(-\mathbf{k}) \neq E_{1,2}(\mathbf{k})$.

Note that quasiparticle dispersion (7) depends on \mathbf{k} not only over the first term under the square root but also over the scalar product depending on quasimomentum polar angle φ . Since vector γ is directed along p_1 axis, $(\gamma\mathbf{p}_F) > 0$ at $|\varphi| < \pi/2$; in the opposite case, $(\gamma\mathbf{p}_F) < 0$.

The energy gap in the spectrum (7) depends on quasimomentum considerably. In particular, it equals to 2Δ at the points of intersection of the FC and p_2 -axis. In the case of $\gamma\mathbf{p}_F > 0$, the gap monotonically increases from 2Δ when polar angle φ between γ and \mathbf{p}_F varies from $\pm\pi/2$ (these points corresponds to $\gamma\mathbf{p}_F = 0$) to zero (if $\varphi = 0$, the gap equals to $2\sqrt{\gamma^2 p_F^2 + \Delta}$).

If $(\gamma\mathbf{p}_F) < 0$, the energy gap is a nonmonotone function of the polar angle. It vanishes at the points of the FC with polar angle $\varphi = \pm\varphi_c$ corresponding to $\gamma\mathbf{p}_F + \Delta = 0$. Thus, if Δ is small enough the spectrum (7) remains gapless. The gap can arise in those directions of the momentum space where the toroidal order parameter exceeds γp_F : $\Delta > \gamma p_F$.

In the case $\Delta < \gamma p_F$, one can expect that Bloch Hamiltonian (5) should be related to a semimetal with insulating gap on some part of the FC corresponding to $-1 < \cos\varphi < -\Delta/\gamma p_F$. Distribution of semimetal and insulating constituents in the real space corresponding to a peculiar intermediate state may be highly complicated. One can think that the phase transition between semimetal and insulating phases should be occurred under the condition that the insulating toroidal order parameter exceeds several critical value, $\Delta > \Delta_c$, where Δ_c can be considered as a minimum value of the toroidal order parameter.

Thus, owing to φ -dependence, the mean field Bloch Hamiltonian (5) describes rather complicated low-temperature insulating phase with toroidal magnetic order. Hamiltonian (5) can be simplified considerably if one replaces scalar product $\gamma\mathbf{p}_F$ with constants corresponding to the averages over the polar angle in the limits of the domains of constant sign of this scalar product, $\gamma\mathbf{p}_F \rightarrow \alpha\gamma_c p_F$. Here $\alpha = \text{sgn}(\gamma\mathbf{p}_F)$, $\gamma_c = \Delta_c/p_F$.

In just the same way as in the case of the Haldane model, mean field Bloch Hamiltonian (5) can be reduced to two independent effective Hamiltonians,

$$\hat{H}_{\alpha\mathbf{k}} = \hbar(\mathbf{v}_F\mathbf{k})\hat{\tau}^3 + [\alpha\gamma_c p_F + \Delta]\hat{\tau}^2, \quad (8)$$

which are distinguished by discrete parameter $\alpha = \pm 1$, which connects the terms breaking space inversion and time reversal symmetries $(\gamma\mathbf{p}_F) + \Delta \rightarrow \alpha\gamma_c p_F + \Delta$.

One can see a direct analogy between the pairs of effective Bloch Hamiltonians corresponding to extremely simplified problem of the excitonic insulator with toroidal magnetic order (8) and the Haldane model [1] described by the effective Hamiltonians (we use somewhat other designations with respect to the original paper [1])

$$\hat{H}_{\alpha\mathbf{k}}^{(0)} = \hbar v_F(k_x\tau^2 - k_y\tau^1) + m_\alpha v_F^2\tau^3 \quad (9)$$

which can be considered as a presentation of a traceless 2×2 matrices in the form of a linear combination of the Pauli matrices. The two effective Hamiltonians (8) coincide with (9) nearly verbally if one considers more general case of the ordering with nonzero both real and imaginal parts of the order parameter, $\Delta = \Delta' + i\Delta'' = |\Delta|e^{i\phi}$. Here, ϕ is a phase of the order parameter ($\phi = \pi/2$ in the case of pure imaginal Δ).

The antipodal directions of quasimomentum, differing with sign of α , turn out to be considerably nonequivalent at $\Delta \neq 0$. Energy gap $E_{g+} = 2(\Delta_c + \Delta)$ is an increasing function of Δ in the case of a direction corresponding to

$\alpha = +1$, whereas the gap $E_{g-} = 2|\Delta_c - \Delta|$ for a direction corresponding to $\alpha = -1$ exhibits a minimum at $\Delta = \Delta_c$ in which $E_{g-} = 0$. Change of sign of the gap corresponds to the band inversion similar to that in the systems with quantum spin Hall effect [6]. It is important that band inversion in excitonic insulator is not a result of the spin-orbit interaction so that one can expect that the Haldane state can be observed at rather high temperature.

Approximate Hamiltonians $\hat{H}_{\alpha\mathbf{k}}$ corresponding to two-band model of excitonic insulator with toroidal magnetic order and effective Hamiltonians $\hat{H}_{\alpha\mathbf{k}}^{(0)}$ of the Haldane model describing 2D honeycomb lattice are not identical. Nevertheless, both $\hat{H}_{\alpha\mathbf{k}}^{(0)}$ and $\hat{H}_{\alpha\mathbf{k}}$ result in the same structure of quasiparticle spectrum. In the case of excitonic insulator we have

$$E_{1,2}^{\alpha}(\mathbf{k}) = \pm \sqrt{\hbar^2(\mathbf{v}_F \mathbf{k})^2 + (\alpha\Delta_c + \Delta)^2}, \quad (10)$$

where the second term under the square root plays role of the mass term m_{α} defined in the Haldane model [1] as

$$m_{\alpha} \equiv M - 3\sqrt{3}\alpha t_2 \sin \phi \rightarrow \alpha\Delta_c + |\Delta| \sin \phi;$$

here $\pm M$ are the energies of the sites of two different sublattices of the honeycomb lattice, t_2 is a matrix element corresponding to the hopping between the second neighbor sites, ϕ is an additional phase corresponding to such a hopping in the Haldane model [1].

Note that triplet electron-hole pairing described by pure imaginal order parameter can be associated with poloidal spin currents in the volume [15] and therefore should be apparent in spin quantum Hall effect. Triplet pairing can be described approximately by the Hamiltonian in the form of a direct sum of two pairs of effective Hamiltonians $\hat{H}_{\mathbf{k}\sigma\alpha}$, similar to (8) or (9), for different spin projections σ , where $\alpha = \pm 1$ for $\sigma = \uparrow$ whereas $\alpha = \mp 1$ for $\sigma = \downarrow$. Similar model was introduced by Bernevig, Huges and Zhang [6] to study the quantum spin Hall effect in HgTe/CdTe quantum wells.

Any Hermitian operator $\hat{H}^{(0)}$ is fully determined by its spectrum E_n and a complete set of eigenfunctions $\psi_{n\nu}$, where quantum number ν takes into account a degeneracy of the eigenvalue E_n . Such a set can be used as an orthonormal basis of the Hilbert space in which operator $\hat{H}^{(0)}$ acts. Let us consider another Hermitian operator \hat{H} acting in the same space and suppose that $\hat{H}^{(0)}$ and \hat{H} have the same spectrum E_n . This fact indicates that the two operators are equivalent,

$$\hat{H} = \hat{U} \hat{H}^{(0)} \hat{U}^{\dagger}, \quad (11)$$

where \hat{U} is a unitary operator. Indeed, a unitary transformation preserves the spectrum in a new orthonormal basis $\hat{U}\psi_{n\nu}$.

Unitary matrix connecting two-band operators (8) and (9) depend on three angle variables, ϑ , θ , φ . Matrix elements can be presented in the form $U_{11} = U_{22}^* = e^{i\vartheta} \cos \varphi$, $U_{12} = -U_{21}^* = e^{i\theta} \sin \varphi$. The explicit form of these matrix elements can be directly obtained from Eq. (11).

One can see that the excitonic insulator with toroidal magnetic order described by the approximate Bloch Hamiltonian (8) and the Haldane model [1] described by the Bloch Hamiltonian (9) are equivalent that is can be related to a class of models in which the Haldane state can be apparent.

To create the Haldane state one needs only the time-reversal symmetry break in 2D crystal. Therefore, it seems that artificial heterostructures in the form of quantum well systems may be the materials in which such a state can be discovered. To obtain desired properties of the electron spectrum of the heterostructure one can easily correct this spectrum by external in-plane magnetic field [16] or by varying of magnetic impurity concentration. We believe that precisely 2D quantum wells with toroidal magnetic order are the most suitable systems to realize the Haldane state.

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- [1] F.D.M. Haldane, Phys. Rev. Lett. **61**, 2015 (1988).
 - [2] G.E. Volovik, Phys. Lett. A **128**, 277 (1988).
 - [3] G.E. Volovik, JETP **67**, 1804 (1988).
 - [4] D.J. Thouless, M. Kohmoto, M.P. Nightingale, and M. den Nijs, Phys. Rev. Lett. **49**, 405 (1982).
 - [5] C.L. Kane and E.J. Mele, Phys. Rev. Lett. **95**, 226801 (2005).
 - [6] B.A. Bernevig, T.L. Hughes, and S-C. Zhang, Science **314**, 1757 (2006).
 - [7] L.V. Keldysh and Yu.V. Kopayev, Sov.Phys. Solid State **6** 2219 (1965).
 - [8] B.A. Volkov, A.A. Gorbatsevich, Yu.V. Kopayev, and V.V. Tugushev, Sov. Phys. JETP **54**, 1008 (1981).
 - [9] N.A. Spaldin, M. Fiebig, and M. Mostovoy, J. Phys.: Condens. Matter **20**, 434203 (2008).
 - [10] V.M. Dubovik and V.V. Tugushev, Phys. Rep. **187**, 145 (1990).
 - [11] A.A. Gorbatsevich, Yu.V. Kopayev, and V.V. Tugushev, Sov. Phys. JETP **58**, 643 (1983).
 - [12] A. Widom, M.H. Friedman, and Y. Srivastava, J. Phys. A: Math. Gen. **19**, L175 (1986).
 - [13] B.I. Halperin and T.M. Rice, Solid State Phys. **21**, 115 (1968).
 - [14] Yu.V. Kopayev, Physics-Uspekhi **52** (11) (2009).
 - [15] A.A. Gorbatsevich and Yu.V. Kopayev, JETP Lett. **39**, 684 (1984).
 - [16] A.A. Gorbatsevich, V.V. Kapaev, and Yu.V. Kopayev, JETP Lett. **57**, 580 (1993).